On the Influence of Uncertainties in Chemical Reaction Rates on Results of the Astrochemical Modelling

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Abstract. With the chemical reaction rate database UMIST95 (Millar etal. 1997) we analyze how uncertainties in rate constants of gas-phase chemical reactions influence the modelling of the molecular abundances in the interstellar medium. Random variations are introduced into the rate constants to estimate the scatter in theoretical abundances. Calculations were performed for the dark and translucent molecular clouds where gas phase chemistry is adequate (Terzieva & Herbst 1998). Similar approach was used by Pineau des Forets & Roueff (2000) for the study of chemical bistability. All the species are divided into 6 sensitivity groups according to the value of the scatter in their model abundances computed with varied rate constants. It is shown that the distribution of species within these groups depends on the number of atoms in them and on the adopted physical conditions. The simple method is suggested which allows to single out reactions that are most important for the evolution of a given species.

1 Scatter in the model abundances

To study the influence of uncertainties in reaction rates on the model abundances we calculated 10^4 variants of each species abundance. Figure 1 shows the scatter for some representative species.

We divided all species into 6 sensitivity groups according to the value of the scatter in their model abundances computed with varied rate constants.

Distribution of the species within these groups depends on adopted physical conditions (see fig. 1). Scatter in logarithmic abundances of simple molecules lies within $0.5 - 1$ dex. Figure 2 shows how the species are distributed by the number of atoms in different sensitivity groups. It is clear that the scatter in abundances significantly increases with the number of atoms in the molecule.

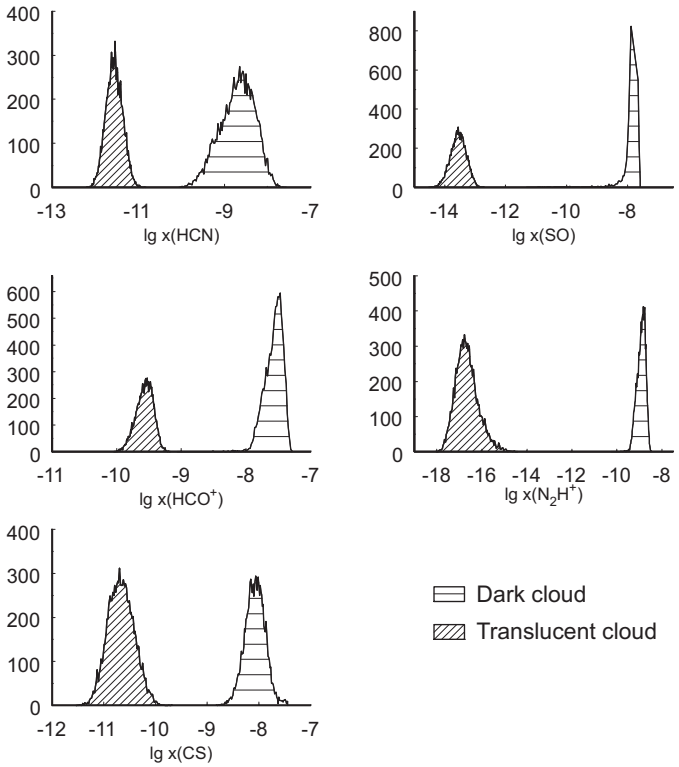

Fig. 1. The distribution of 10000 model abundances calculated with different rate coefficients

As an example we considered two molecules, HCN and C_2S, which in the gas-phase chemistry reach maximum of their abundance at about 10^4 years and, hence, considered to be characteristic representatives of the "early" chemistry. For example, high abundances of HC_3N and other cyanopolyynes in the dark cloud TMC-1 are considered to prove that this object is chemically young (Hirahara etal. 1992).

Our calculations show that in the dark cloud model HC_3N and C_2S molecules belong to the sensitivity group 4, while more complex cyanopolyynes (HC_5N, etc.) fall in the groups 5 and 6.

Left panel of fig.3 displays time dependence of the HC_3N abundance calculated with the sets of constants providing maximal, minimal and 2 intermediate equilibrium abundances. It is clear that variations of the equilibrium HC_3N abundance are accompanied by noticeable changes of the time when the maximal abundance is achieved (from $7{\cdot}10^4$ to $3{\cdot}10^5$ yr). The right panel displays corresponding dependence for C_2S. The peak in the C_2S abundance time dependence is more flat and shifts less. Anyhow, quantitative estimates of the molecular cloud ages on the basis of molecular abundances and their

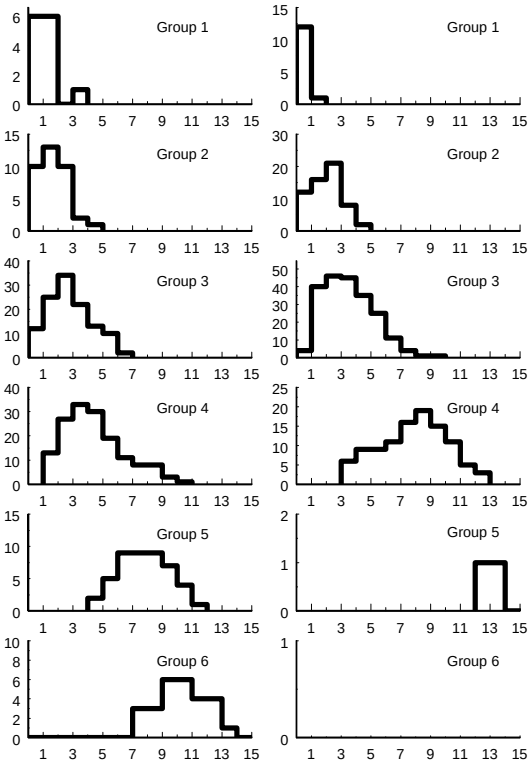

Fig. 2. Distribution of the molecules by number of atoms for different sensitivity groups. Left column – dark cloud, right column – translucent cloud

ratios (as suggested in, e.g., in Stahler 1984) are subject to this additional uncertainty.

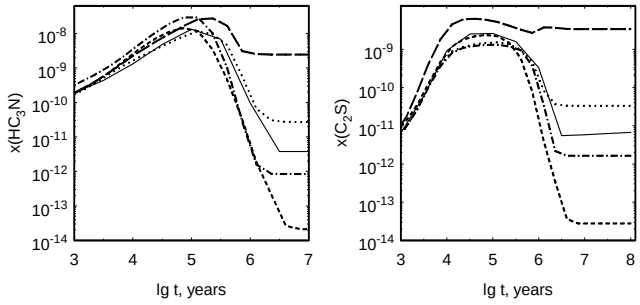

Fig. 3. Evolution of the HC_3N and C_2S abundances calculated with different rate coefficients

2 Correlation between the species abundance and reaction rate constant

Because of nonlinearity of the rate equations it is impossible to sort out analytically the reactions which rate uncertainty greatly affects the total uncertainty of a species abundance. We propose a simple statistical method to resolve the issue. The method is based on investigation of correlations between the species abundance and rate constants of the reactions and allows to estimate how the increased precision of the reaction rate constant will decrease the uncertainty in the species abundance.

Figure 4 shows distribution of HCO^+ abundances in the plane "rate coefficient – abundance". The left panel represents the coverage of the plane for reaction with the large correlation coefficient H_2 + C.R.P. $\rightarrow$ H_2^+ + e^- ($r = 0.84$) and the right panel – that for reaction with the small coefficient C + NH $\rightarrow$ CH + N ($r = 0.01$). Additional modelling makes possible to predict improvement of the abundance estimate for the case when rates of several reactions are going to be remeasured.

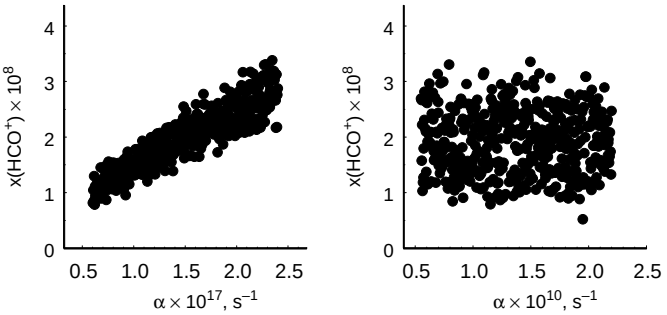

Fig. 4. HCO^+ model abundances in the "rate coefficient-abundance" plane

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